

Ethyl 2-ethyl-3-hydroxybutanoate  
5465-11-2 | DTXSID90282959

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 217 °C

Global applicability domain: Inside

Local applicability domain index: 6.78e-01

Confidence level: 7.76e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Isopentyl lactate</div> <div>Measured: 202</div> <div>Predicted: 205</div>	<div>Image not found</div> <div>Diethylene glycol monoisobutyl ether</div> <div>Measured: 217</div> <div>Predicted: 219</div>	<div>Image not found</div> <div>2-(2-Butoxyethoxy)ethanol</div> <div>Measured: 231</div> <div>Predicted: 228</div>
<div>Image not found</div> <div>2-[2-(2-Methoxyethoxy)ethoxy]ethanol</div> <div>Measured: 249</div> <div>Predicted: 243</div>	<div>Image not found</div> <div>Butyl lactate</div> <div>Measured: 186</div> <div>Predicted: 184</div>	